

chain nodes :

9	10	11	14	15	18	25	26	27	28	29	30	31	32	33	34	40	41	42	43	55	56	57
58	59	60	61	62	63	64	65	66	67	69	70	71	72	73	74	75	91	92	93	94	95	

ring nodes :

1	2	3	4	5	6	19	20	21	22	23	24	35	36	37	38	39	44	45	46	47	48	76	77
78	79	80	81	82	83	84	85	86	87	88	89	90											

chain bonds :

3-9	5-55	9-10	10-11	11-14	14-15	18-19	18-25	26-27	27-28	29-30	29-31	30-32										
32-33	34-35	36-42	37-41	39-40	43-44	56-57	56-59	56-63	57-58	60-61	60-64	61-62										
65-66	65-69	65-70	66-67	71-72	71-73	74-75	78-91	79-93	84-95	88-92	89-94											

ring bonds :

1-2	1-6	2-3	3-4	4-5	5-6	19-20	19-24	20-21	21-22	22-23	23-24	35-36	35-39	36-37								
37-38	38-39	44-45	44-48	45-46	46-47	47-48	76-77	76-80	77-78	78-79	79-80	81-82										
81-85	82-83	83-84	84-85	86-87	86-90	87-88	88-89	89-90														

exact/norm bonds :

3-9	5-55	14-15	18-19	19-20	19-24	20-21	21-22	22-23	23-24	29-30	30-32	35-36										
35-39	36-37	37-38	38-39	44-45	44-48	45-46	46-47	47-48	56-57	56-59	56-63	60-61										
60-64	65-66	65-69	65-70	66-67	71-72	74-75	76-77	76-80	77-78	78-79	79-80	79-93										
81-82	81-85	82-83	83-84	84-85	84-95	86-87	86-90	87-88	88-89	89-90	89-94											

exact bonds :

9-10	10-11	11-14	18-25	26-27	27-28	29-31	32-33	34-35	36-42	37-41	39-40	43-44										
57-58	61-62	71-73	78-91	88-92																		

normalized bonds :

1-2	1-6	2-3	3-4	4-5	5-6
-----	-----	-----	-----	-----	-----

isolated ring systems :
containing 1 :

G1:C,N

G2:[*1],[*2],[*3],[*4],[*5]

G3:H,Cy,Ak

G4:[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 9:CLASS 10:CLASS 11:CLASS 14:CLASS
15:CLASS 18:CLASS 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:CLASS
26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS
35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:CLASS 41:CLASS 42:CLASS 43:CLASS
44:Atom 45:Atom 46:Atom 47:Atom 48:Atom 55:CLASS 56:CLASS 57:CLASS 58:CLASS
59:CLASS 60:CLASS 61:CLASS 62:CLASS 63:Atom 64:Atom 65:CLASS 66:CLASS 67:CLASS
69:CLASS 70:CLASS 71:CLASS 72:CLASS 73:CLASS 74:CLASS 75:CLASS 76:Atom 77:Atom
78:Atom 79:Atom 80:Atom 81:Atom 82:Atom 83:Atom 84:Atom 85:Atom 86:Atom 87:Atom
88:Atom 89:Atom 90:Atom 91:CLASS 92:CLASS 93:Atom 94:Atom 95:Atom

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=> file reg
COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE TOTAL
ENTRY SESSION
0.21 0.21

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=>Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END) :end

=>
Uploading C:\STNEXP4\QUERIES\10046616.str

L1 STRUCTURE uploaded

=> que L1

L2 QUE L1

=> d l1
L1 HAS NO ANSWERS
L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss sam
SAMPLE SEARCH INITIATED 11:07:51 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 153 TO ITERATE

100.0% PROCESSED 153 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 2318 TO 3802
PROJECTED ANSWERS: 0 TO 0

L3 0 SEA SSS SAM L1

10046616

V. Balasubramanian

=> log y
COST IN U.S. DOLLARS
FULL ESTIMATED COST

SINCE FILE ENTRY	TOTAL SESSION
0.40	0.61

Connection closed by remote host

10046616

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=>Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

=>
Uploading C:\STNEXP4\QUERIES\10046616.str

L1 STRUCTURE uploaded

=> que L1

L2 QUE L1

=> d l1
L1 HAS NO ANSWERS
L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss sam
SAMPLE SEARCH INITIATED 11:03:45 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 146 TO ITERATE

100.0% PROCESSED 146 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 2196 TO 3644
PROJECTED ANSWERS: 0 TO 0

10/046,616

V. Balasubramanian

L3 0 SEA SSS SAM L1

=> s 11 sss ful
FULL SEARCH INITIATED 11:04:25 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 2984 TO ITERATE

100.0% PROCESSED 2984 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L4 0 SEA SSS FUL L1

STN INTERNATIONAL LOGOFF AT 11:04:32 ON 24 NOV 2003

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LOGINID: ssspta1611bxv

PASSWORD:
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Uploading C:\STNEXP4\QUERIES\10046616.str

L1 STRUCTURE UPLOADED

=> que L1

L2 OUE L1

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=> d 11
L1 HAS NO ANSWERS
L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

```
=> s 11 sss sam
SAMPLE SEARCH INITIATED 11:07:51 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      153 TO ITERATE
```

100.0% PROCESSED 153 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

| | | |
|------------------------|---------|--------------|
| FULL FILE PROJECTIONS: | ONLINE | **COMPLETE** |
| | BATCH | **COMPLETE** |
| PROJECTED ITERATIONS: | 2318 TO | 3802 |
| PROJECTED ANSWERS: | 0 TO | 0 |

L3 0 SEA SSS SAM L1

Connection closed by remote host

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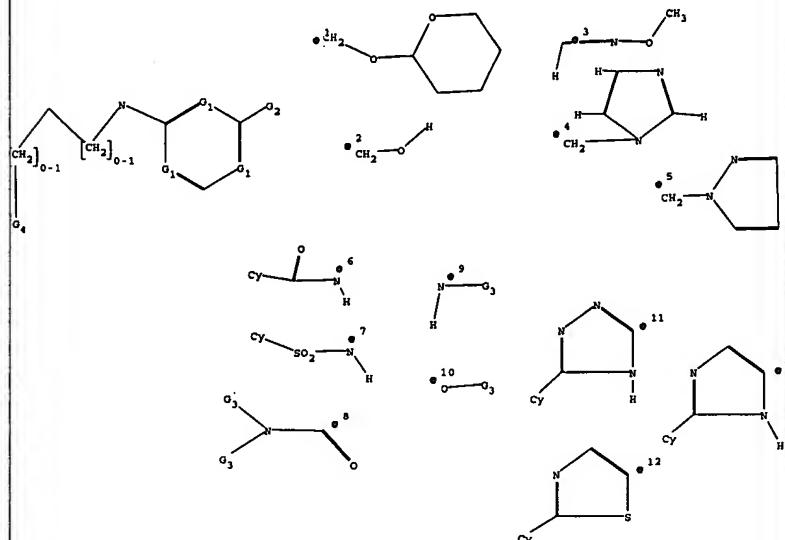
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
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361



chain nodes :

| | | | | | | | | | | | | | | | | | | | | | | |
|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|
| 9 | 10 | 11 | 14 | 15 | 18 | 25 | 26 | 27 | 28 | 29 | 30 | 31 | 32 | 33 | 34 | 40 | 41 | 42 | 43 | 55 | 56 | 57 |
| 58 | 59 | 60 | 61 | 62 | 63 | 64 | 65 | 66 | 67 | 69 | 70 | 71 | 72 | 73 | 74 | 75 | 91 | 92 | 93 | 94 | 95 | |

ring nodes :

| | | | | | | | | | | | | | | | | | | | | | | | |
|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|
| 1 | 2 | 3 | 4 | 5 | 6 | 19 | 20 | 21 | 22 | 23 | 24 | 35 | 36 | 37 | 38 | 39 | 44 | 45 | 46 | 47 | 48 | 76 | 77 |
| 78 | 79 | 80 | 81 | 82 | 83 | 84 | 85 | 86 | 87 | 88 | 89 | 90 | | | | | | | | | | | |

chain bonds :

| | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| 3-9 | 5-55 | 9-10 | 10-11 | 11-14 | 14-15 | 18-19 | 18-25 | 26-27 | 27-28 | 29-30 | 29-31 | 30-32 |
| 32-33 | 34-35 | 36-42 | 37-41 | 39-40 | 43-44 | 56-57 | 56-59 | 56-63 | 57-58 | 60-61 | 60-64 | 61-62 |
| 65-66 | 65-69 | 65-70 | 66-67 | 71-72 | 71-73 | 74-75 | 78-91 | 79-93 | 84-95 | 88-92 | 89-94 | |

ring bonds :

| | | | | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|--|
| 1-2 | 1-6 | 2-3 | 3-4 | 4-5 | 5-6 | 19-20 | 19-24 | 20-21 | 21-22 | 22-23 | 23-24 | 35-36 | 35-39 | 36-37 | |
| 37-38 | 38-39 | 44-45 | 44-48 | 45-46 | 46-47 | 47-48 | 76-77 | 76-80 | 77-78 | 78-79 | 79-80 | 81-82 | | | |
| 81-85 | 82-83 | 83-84 | 84-85 | 86-87 | 86-90 | 87-88 | 88-89 | 89-90 | | | | | | | |

exact/norm bonds :

| | | | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| 1-2 | 1-6 | 2-3 | 3-4 | 3-9 | 4-5 | 5-6 | 5-55 | 9-10 | 10-11 | 11-14 | 14-15 | 18-19 | 18-25 | 19-20 |
| 19-24 | 20-21 | 21-22 | 22-23 | 23-24 | 26-27 | 27-28 | 29-30 | 29-31 | 30-32 | 32-33 | 34-35 | 35-36 | | |
| 35-39 | 36-37 | 36-42 | 37-38 | 37-41 | 38-39 | 39-40 | 43-44 | 44-45 | 44-48 | 45-46 | 46-47 | 47-48 | | |
| 56-57 | 56-59 | 56-63 | 57-58 | 60-61 | 60-64 | 61-62 | 65-66 | 65-69 | 65-70 | 66-67 | 71-72 | 71-73 | | |
| 74-75 | 76-77 | 76-80 | 77-78 | 78-79 | 78-91 | 79-80 | 79-93 | 81-82 | 81-85 | 82-83 | 83-84 | 84-85 | | |
| 84-95 | 86-87 | 86-90 | 87-88 | 88-89 | 88-92 | 89-90 | 89-94 | | | | | | | |

isolated ring systems :

containing 1 :

G1:C,N

G2:[*1],[*2],[*3],[*4],[*5]

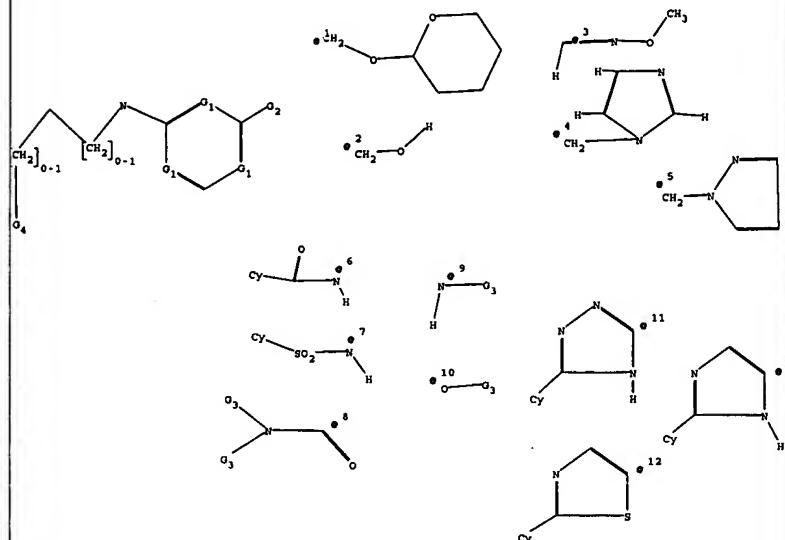
G3:H,Cy,Ak

G4:[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 9:CLASS 10:CLASS 11:CLASS 14:CLASS
15:CLASS 18:CLASS 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:CLASS
26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS
35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:CLASS 41:CLASS 42:CLASS 43:CLASS
44:Atom 45:Atom 46:Atom 47:Atom 48:Atom 55:CLASS 56:CLASS 57:CLASS 58:CLASS
59:CLASS 60:CLASS 61:CLASS 62:CLASS 63:Atom 64:Atom 65:CLASS 66:CLASS 67:CLASS
69:CLASS 70:CLASS 71:CLASS 72:CLASS 73:CLASS 74:CLASS 75:CLASS 76:Atom 77:Atom
78:Atom 79:Atom 80:Atom 81:Atom 82:Atom 83:Atom 84:Atom 85:Atom 86:Atom 87:Atom
88:Atom 89:Atom 90:Atom 91:CLASS 92:CLASS 93:Atom 94:Atom 95:Atom

261



chain nodes :

| | | | | | | | | | | | | | | | | | | | | | | |
|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|
| 9 | 10 | 11 | 14 | 15 | 18 | 25 | 26 | 27 | 28 | 29 | 30 | 31 | 32 | 33 | 34 | 40 | 41 | 42 | 43 | 55 | 56 | 57 |
| 58 | 59 | 60 | 61 | 62 | 63 | 64 | 65 | 66 | 67 | 69 | 70 | 71 | 72 | 73 | 74 | 75 | 91 | 92 | 93 | 94 | 95 | |

ring nodes :

| | | | | | | | | | | | | | | | | | | | | | | | |
|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|
| 1 | 2 | 3 | 4 | 5 | 6 | 19 | 20 | 21 | 22 | 23 | 24 | 35 | 36 | 37 | 38 | 39 | 44 | 45 | 46 | 47 | 48 | 76 | 77 |
| 78 | 79 | 80 | 81 | 82 | 83 | 84 | 85 | 86 | 87 | 88 | 89 | 90 | | | | | | | | | | | |

chain bonds :

| | | | | | | | | | | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|--|--|--|--|--|--|--|--|--|
| 3-9 | 5-55 | 9-10 | 10-11 | 11-14 | 14-15 | 18-19 | 18-25 | 26-27 | 27-28 | 29-30 | 29-31 | 30-32 | | | | | | | | | |
| 32-33 | 34-35 | 36-42 | 37-41 | 39-40 | 43-44 | 56-57 | 56-59 | 56-63 | 57-58 | 60-61 | 60-64 | 61-62 | | | | | | | | | |
| 65-66 | 65-69 | 65-70 | 66-67 | 71-72 | 71-73 | 74-75 | 78-91 | 79-93 | 84-95 | 88-92 | 89-94 | | | | | | | | | | |

ring bonds :

| | | | | | | | | | | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|--|--|--|--|--|--|--|
| 1-2 | 1-6 | 2-3 | 3-4 | 4-5 | 5-6 | 19-20 | 19-24 | 20-21 | 21-22 | 22-23 | 23-24 | 35-36 | 35-39 | 36-37 | | | | | | | |
| 37-38 | 38-39 | 44-45 | 44-48 | 45-46 | 46-47 | 47-48 | 76-77 | 76-80 | 77-78 | 78-79 | 79-80 | 81-82 | | | | | | | | | |
| 81-85 | 82-83 | 83-84 | 84-85 | 86-87 | 86-90 | 87-88 | 88-89 | 89-90 | | | | | | | | | | | | | |

exact/norm bonds :

| | | | | | | | | | | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|--|--|--|--|--|--|--|
| 1-2 | 1-6 | 2-3 | 3-4 | 3-9 | 4-5 | 5-6 | 5-55 | 9-10 | 10-11 | 11-14 | 14-15 | 18-19 | 18-25 | 19-20 | | | | | | | |
| 19-24 | 20-21 | 21-22 | 22-23 | 23-24 | 26-27 | 27-28 | 29-30 | 29-31 | 30-32 | 32-33 | 34-35 | 35-36 | | | | | | | | | |
| 35-39 | 36-37 | 36-42 | 37-38 | 37-41 | 38-39 | 39-40 | 43-44 | 44-45 | 44-48 | 45-46 | 46-47 | 47-48 | | | | | | | | | |
| 56-57 | 56-59 | 56-63 | 57-58 | 60-61 | 60-64 | 61-62 | 65-66 | 65-69 | 65-70 | 66-67 | 71-72 | 71-73 | | | | | | | | | |
| 74-75 | 76-77 | 76-80 | 77-78 | 78-79 | 78-91 | 79-80 | 79-93 | 81-82 | 81-85 | 82-83 | 83-84 | 84-85 | | | | | | | | | |
| 84-95 | 86-87 | 86-90 | 87-88 | 88-89 | 88-92 | 89-90 | 89-94 | | | | | | | | | | | | | | |

isolated ring systems :

containing 1 :

G1:C,N

G2:[*1],[*2],[*3],[*4],[*5]

G3:H,Cy,Ak

G4:[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 9:CLASS 10:CLASS 11:CLASS 14:CLASS
15:CLASS 18:CLASS 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:CLASS
26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS
35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:CLASS 41:CLASS 42:CLASS 43:CLASS
44:Atom 45:Atom 46:Atom 47:Atom 48:Atom 55:CLASS 56:CLASS 57:CLASS 58:CLASS
59:CLASS 60:CLASS 61:CLASS 62:CLASS 63:Atom 64:Atom 65:CLASS 66:CLASS 67:CLASS
69:CLASS 70:CLASS 71:CLASS 72:CLASS 73:CLASS 74:CLASS 75:CLASS 76:Atom 77:Atom
78:Atom 79:Atom 80:Atom 81:Atom 82:Atom 83:Atom 84:Atom 85:Atom 86:Atom 87:Atom
88:Atom 89:Atom 90:Atom 91:CLASS 92:CLASS 93:Atom 94:Atom 95:Atom

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LOGINID:ssspta1611bxv

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

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NEWS WWW CAS World Wide Web Site (general information)

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FILE 'HOME' ENTERED AT 10:48:11 ON 24 NOV 2003

| => file reg | SINCE FILE | TOTAL |
|----------------------|------------|---------|
| COST IN U.S. DOLLARS | ENTRY | SESSION |
| FULL ESTIMATED COST | 0.21 | 0.21 |

FILE 'REGISTRY' ENTERED AT 10:48:20 ON 24 NOV 2003

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TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=>Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

=>
Uploading C:\STNEXP4\QUERIES\10046616.str

L1 STRUCTURE UPLOADED

=> que L1

L2 QUE L1

=> d 12

L2 HAS NO ANSWERS

L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

L2 QUE L1

=> s l1 sss sam

SAMPLE SEARCH INITIATED 10:48:57 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 603776 TO ITERATE

0.2% PROCESSED 1000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: EXCEEDS 1000000
PROJECTED ANSWERS: EXCEEDS 0

L3 0 SEA SSS SAM L1

10046616

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=> log y
COST IN U.S. DOLLARS
FULL ESTIMATED COST

| SINCE FILE ENTRY | TOTAL SESSION |
|------------------|---------------|
| 0.40 | 0.61 |

STN INTERNATIONAL LOGOFF AT 10:49:12 ON 24 NOV 2003

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Welcome to STN International! Enter x:x

LOGINID:ssspta1611bxv

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

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FILE 'HOME' ENTERED AT 10:54:12 ON 24 NOV 2003

=> file reg
COST IN U.S. DOLLARS
FULL ESTIMATED COST

| SINCE FILE ENTRY | TOTAL SESSION |
|------------------|---------------|
| 0.21 | 0.21 |

FILE 'REGISTRY' ENTERED AT 10:54:22 ON 24 NOV 2003

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<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=>Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

=>
Uploading C:\STNEXP4\QUERIES\10046616.str

L1 STRUCTURE uploaded

=> que L1

L2 QUE L1

=> d 11
L1 HAS NO ANSWERS
L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s 11 sss sam
SAMPLE SEARCH INITIATED 10:55:00 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 62234 TO ITERATE

1.6% PROCESSED 1000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: EXCEEDS 1000000
PROJECTED ANSWERS: EXCEEDS 0

L3 0 SEA SSS SAM L1

10046616

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| | | |
|----------------------|------------|---------|
| => log.y | | |
| COST IN U.S. DOLLARS | SINCE FILE | TOTAL |
| | ENTRY | SESSION |
| FULL ESTIMATED COST | 0.40 | 0.61 |

STN INTERNATIONAL LOGOFF AT 10:55:05 ON 24 NOV 2003

10046616